

Recent Advances in the Application of Synchrotron Radiation to Catalysis Workshop

May 22, 2002

In a successful and informative workshop titled "Recent Advances in the Application of Synchrotron Radiation to Catalysis," topics ranged from new developments of using soft x-rays at high pressures to in situ X-Ray Diffraction (XRD) studies.

Chemist Gary Haller, of Yale University, began the workshop with a talk on a detailed characterization of platinum and tin in PtSn-MCM41 catalysts.



Workshop Participants

Simon Bare, from UOP LLC - a leading company in developing and commercializing technology for license to the oil refining, petrochemical and gas processing industries, headquartered in Des Plaines, Illinois - showed how theoretical calculations combined with in situ X-ray Absorption Near-Edge Structure (XANES) is a powerful combination that provided detailed insight into the chemistry of small platinum clusters.

Chemical engineer Enrique Iglesia, from the University of California, Berkeley, showed several examples highlighting both the power and also the drawbacks of X-ray Absorption Fine Structure (XAFS) in catalyst characterization, particularly in supported metal oxide catalysts. He emphasized the need that the characterization must be combined with catalyst activity in order to ensure that meaningful structure-activity relationships are developed.

BNL chemist Jon Hanson highlighted the applicabil-

ity of in situ X-Ray Diffraction (XRD) for following structural phase transformation in bulk catalysts.

The applicability of Near-Edge X-ray Absorption Fine Structure (NEXAFS) to characterize the electronic structure of both model and real catalysts was demonstrated by Jingguang Chen, of the University of Delaware in Newark.

Chemist Robert Schloegl, of Fritz-Haber-Institute in Berlin, Germany, updated the workshop on recent developments in using soft x-rays at more realistic reaction conditions to probe the electronic structure and chemical form of the surfaces of working catalysts. He showed two examples where the activity of the catalyst was linked to a particular species that was only present under reaction conditions, this highlighting the need for in situ surface sensitive spectroscopy.

Chemical engineer and materials scientist Daniel Resasco, of the University of Oklahoma in Tulsa, talked about a novel catalyst used for producing single-walled carbon nanotubes, and how Extended X-ray Absorption Fine Structure (EXAFS) was critical in developing an understanding the structure of the active form of the catalyst.

John Gland, of the University of Michigan in Ann Arbor, used in situ Fluorescence Yield Near Edge Spectroscopy (FYNES) to not only characterize the intermediates present during the total oxidation of hydrocarbons on single crystals of platinum but also to follow the kinetics of the oxidation.

BNL chemist Jan Hrbek closed out the workshop with a talk on the use of high resolution X-ray Photoelectron Spectroscopy (XPS), combined with Density Functional Theory (DFT) calculations, to follow the sulfidation of a titanium dioxide single crystal surface.
-Simon Bare